One-Dimensional Exactly Solvable Model of Polaron

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Abstract

Using for unperturbed electron and phonon Hamiltonians a representation by the Jacobi matrices a one-dimensional model of the electron-phonon interaction is constructed. In frame of the model the polaron and scattering spectral bands are calculated explicitly as well as the corresponding states. An explicit formula for the polaron effective mass is derived and the fit of model parameters is suggested. A connection of the model with the description of phonon degrees of freedom for quantum wires is discussed.

1 Introduction

The physical motivation of the present paper is that even for quantum description of the simplest nanoelectronic devices (like a quantum wire) one have to take into account the interaction of the propagating electron with the internal degrees of freedom of the device. This interaction becomes valuable in the case for instance, when the voltage applied is large enough or the temperature of the device is high. The simplest excitations in both cases are phonons. It means that the first step in the correct description of any nanoelectronic device at nonzero temperature or at large voltage applied is taking into account the electron phonon-interaction. This leads to polarons as charge carriers instead of electrons. In general the effective mass of polaron is greater than the one of electron in the lattice. So one of the important problem is to calculate the effective mass of charge carriers and to estimate its contribution into the physical characteristics of the working regime of the device.

The standard field theoretical models the electron-phonon interaction such as Frölich model [1] do not preserve the number of particles and cannot be solved explicitly. This makes interesting the construction of the phenomenological models of electron-phonon interaction with fixed number of particles. The first step in this direction is the study of two-particle models (one electron interacts with one phonon).

The first attempt to construct such a model was undertaken in the paper [2] where the electron was described by the one-dimensional Schrödinger operator with the Krönig-Penny potential and phonon was described by the Jacobi matrix. The interaction in this model is localized on the diagonal of electron-phonon space. Being exactly solvable this model however is not able to calculate explicitly the effective masses of the quasiparticle aroused. The physical difficulty related to this model is the difference of scales introduced for description of phonon and electron (continuous configuration space for electron and the lattice for phonon).

In the present paper we describe and solve a similar model where the kinetic energy operators are given by Jacobi matrices for both electron and phonon. This makes possible to calculate explicitly the eigenfunctions of the polaron branch of spectrum and corresponding effective masses. Another simplification in comparison to the model from [2] is that we take into account the influence of the lattice potential on the electron by changing of its mass by the effective one in the kinetic energy operator.

2 Model

We start with the one-dimensional lattice $\mathbf{Z}$. Set $H = l^2(\mathbf{Z})$ be the state space of a quantum particle on the lattice and T be the unitary shift operator in H, $(T\varphi)_n = \varphi_{n-1}$. Introduce the unperturbed phonon and electron hamiltonians on H as $L_1 = T + T^*$ and $L_2 = \xi(T + T^*)$ respectively. Here the real parameter ξ makes sense of ratio $\xi \sim \frac{\hbar\omega_0}{E_{char}}$ up to a dimensionless factor where ω_0 is the frequency of the lattice oscillations and E_{char} is a characteristic scale of the electron energy i.e. the width of conductivity zone. The hamiltonian of electron-phonon system without interaction acts in $\mathcal{H} = H \otimes H = l^2(\mathbf{Z}^2)$ as $L_0 = L_1 \otimes I + I \otimes L_2$. Its spectrum is given by $\sigma(L_0) = \overline{\sigma(L_1) + \sigma(L_2)} = [-2(1 + |\xi|), 2(1 + |\xi|)]$.

We will suppose that the lattice is homogeneous and the interaction between electron and phonon is localized. This restricts the choice of the interaction operator V, $L = L_0 + V$

being the perturbed hamiltonian by the following assumptions.

Assumption 1. .

$[V, R] = 0$, where $(Rg)_{m,n} = g_{m+1,n+1}$ is the operator of the electron-phonon shift in $\mathcal{H}$, - space homogeneity.

Assumption 2.

$\forall n \in \mathbf{Z}$ $g_{n,n} = 0$ implies $Vg = 0$, - locality.

The locality assumption means that V differs from zero on the main diagonal $\mathcal{D} = \{g \in l^2(\mathbf{Z}^2) : \ g_{mn} = 0 \text{ for } m \neq n\}$ of $l^2(\mathbf{Z}^2)$ only. By the assumption **1** it commutes on $\mathcal{D}$ with the shift operator. Thus V is given just by convolution with a function $\Psi \in l^\infty(\mathbf{Z})$,

$$(Vg)_{n,m} = \delta_{n,m} \sum_{\tau \in \mathbf{Z}} \Psi_\tau g_{n-\tau,n-\tau}.$$

Assuming the symmetricity of V one gets $\Psi_\tau = \overline{\Psi_{-\tau}}$. If Ψ_τ is well-behaved (for instance if $\sum_\tau |\Psi_\tau| < \infty$ and so V is bounded) then V is selfadjoint. Generally one can define the selfadjoint operator V in $\mathcal{D} \simeq l^2(\mathbf{Z})$ as the Fourier transform of the operator of multiplication on real valued function $\Psi(p) = \sum_\tau \Psi_\tau e^{ip\tau}$ in $L^2[-\pi, \pi]$.

2.1 Spectrum of the Operator L

To study operator L it is convenient to use the spectral representation of R given by the Gelfand transform $\mathcal{F} : \ l^2(\mathbf{Z}^2) \to L^2([-\pi, \pi], l^2(\mathbf{Z})) \equiv \widetilde{\mathcal{H}}$,

$$(\mathcal{F}g)_s(\kappa) = \frac{1}{\sqrt{2\pi}} \sum_n g_{s+n,n} e^{i\kappa n}.$$

Properties of $\mathcal{F}$

1°. $\mathcal{F}$ is isometric surjection.

Proof

Set $D_s = \{g_{n,m} \neq 0 \Longrightarrow n - m = s\}$ hence $D_s \perp D_{s'}$ for $s \neq s'$ and $\mathcal{H} = \oplus_{s \in \mathbf{Z}} D_s$. Denote as $\widetilde{D}_s = \mathcal{F}D_s \equiv L^2(-\pi, \pi)e_s$, e_s being the s-th element of the standard basis in $l^2(\mathbf{Z})$. We see that $\widetilde{D}_s \perp \widetilde{D}_{s'}$ for $s \neq s'$ and $\widetilde{\mathcal{H}} = \oplus \widetilde{D}_s$. Then $\mathcal{F}|_{D_s}$ is just usual Fourier transform. Thus $\mathcal{F}|_{D_s}$ is surjective isometry. •

2°. $\mathcal{F}$ diagonalizes R, $R = \mathcal{F}^{-1} e^{i\kappa} \cdot \mathcal{F}$.

3°. $L_0 = \mathcal{F}^{-1} \widetilde{L}_0 \mathcal{F}$ where $\widetilde{L}_0 = \int_{-\pi}^{\pi} \oplus \widetilde{L}_0(\kappa) d\kappa$ and

$$\widetilde{L}_0(\kappa) = (\xi + e^{-i\kappa})T + (\xi + e^{i\kappa})T^*$$

We remind that T is the shift operator in $l^2(\mathbf{Z})$.

4°. $\mathcal{F}$ diagonalizes V, $V = \mathcal{F}^{-1} \widetilde{V} \mathcal{F}$, where

$$(\widetilde{V}g)_s(\kappa) = \delta_{s,0} \Psi(\kappa) g_s(\kappa).$$

Proof

Since D_s are invariant subspaces of R and $\mathcal{F}$ the property 2° expresses the fact that shift turns to multiplication on function $e^{i\kappa}$ under the Fourier transform. This together with commutation of $\mathcal{F}$ with the shift on s-variable implies 3°. The property 4° expresses the fact that under the Fourier transform the convolution becomes operator of multiplication on function. •

Thus $\widetilde{L} = \widetilde{L}_0 + \widetilde{V}$ is partially diagonalized by $\mathcal{F}$ i.e.

$$\widetilde{L} = \int_{-\pi}^{\pi} \oplus \widetilde{L}(\kappa) d\kappa,$$

$$\widetilde{L}(\kappa) = (\xi + e^{-i\kappa})T + (\xi + e^{i\kappa})T^* + \Psi(\kappa)P_0$$

where $(P_0\varphi)_s = \delta_{s,0}\varphi_s$ is the projection in the fibre $l^2(\mathbf{Z})$.

Since $\widetilde{L}(\kappa)$ is the rank one perturbation of the standard Jacobi matrix we have $\sigma_c(L_\kappa) = [-2\left|\xi + e^{i\kappa}\right|, 2\left|\xi + e^{i\kappa}\right|]$. This spectrum corresponds to scattered waves type eigenfunctions of L. It fills the zone

$$\sigma_{sc.\,wave} = \bigcup_{\kappa\in[-\pi,\pi]} \sigma_c\left(\widetilde{L}(\kappa)\right) = [-2\left(1 + |\xi|\right), 2\left(1 + |\xi|\right)]$$

which coincides with the spectrum of unperturbed operator L_0.

2.2 Polaron

We are now interested in the waveguide type eigenfunctions of continuous spectrum of L, i.e. those which satisfy the condition $\varphi_{n,m} = O\left(\exp(-C|n-m|)\right)$. In physical literature such eigenfunctions are called polarons. It follows from the previous section that polarons with definite lengthwise momentum $\kappa \in [-\pi, \pi]$ i.e. satisfying the condition $R\varphi = \chi\varphi$, $\chi = e^{i\kappa}$ correspond to l^2-eigenfunctions of $\widetilde{L}(\kappa)$. This reduces the spectral problem $\widetilde{L}(\kappa)\varphi = \lambda\varphi$ to the one for Jacobi matrix

$$Q_\chi = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots & & \\ \cdots & 0 & \xi+\chi & 0 & \cdots & \\ \cdots & \xi+\overline{\chi} & \Psi(\kappa) & \xi+\chi & 0 & \cdots \\ \cdots & 0 & \xi+\overline{\chi} & 0 & \xi+\chi & 0 \\ & \cdots & 0 & \xi+\overline{\chi} & 0 & \xi+\chi \\ & & \cdots & 0 & \xi+\overline{\chi} & 0 \\ & & & \cdots & 0 & \cdots \end{pmatrix}$$

or

$$(Q_\chi\varphi)_n = (\xi+\overline{\chi})\varphi_{n-1} + (\xi+\chi)\varphi_{n+1},\ n \neq 0$$
$$(Q_\chi\varphi)_0 = (\xi+\overline{\chi})\varphi_{-1} + \Psi(\kappa)\varphi_0 + (\xi+\chi)\varphi_1.$$

Note that

$$U_\kappa^*\widetilde{L}(\kappa)U_\kappa = |\xi+\chi|\left(J + \hat{V}\right)$$

where

$$U_\kappa = \mathrm{diag}\ \left\{e^{in\tau}\right\}_{n\in\mathbf{Z}}, \qquad \tau = \arg(\xi+\chi), \quad J_{i,j} = \delta_{i,j+1} + \delta_{i,j-1}$$

and

$$\hat{V} = \frac{\Psi(\kappa)}{|\xi+\chi|}P_0.$$

Thus the l^2-eigenfunction of Q_χ corresponds to the eigenvalue $\lambda = |\xi+\chi|\left(a + a^{-1}\right)$ given by solution of the secular equation

$$a^2 + \frac{\Psi(\kappa)}{|\xi+\chi|}a - 1 = 0 \tag{1}$$

with $|a| < 1$. Solving this equation one gets that the polaron energy λ is related to κ through the dispersion relation

$$\lambda(\kappa) = \mathrm{sign}\Psi(\kappa)\ \sqrt{\Psi(\kappa)^2 + 4(1 + \xi^2 + 2\xi\cos\kappa)}. \tag{2}$$

The corresponding eigenfunction of $\widetilde{L}(\kappa)$ has the form

$$\varphi_n(\kappa, \lambda) = e^{in\tau}a^{|n|}.$$

Note that equation (2) shows that in the case of strong coupling ($\Psi(\kappa) \gg 1$) the polaron zone is separated from spectrum corresponding to the scattered waves. For the small coupling $\Psi(\kappa) \sim 0$ the polaron zone and $\sigma_{sc.\,wave}$ are overlapped. Note however that the polaron decay is impossible for the energies belonging to the common part of spectrum. This is the result of high common symmetry of L and L_0 provided by R.

For completeness we now right down the generalized eigenfunctions of $\widetilde{L}(\kappa)$ scattered waves type. The solution of the equation $\widetilde{L}(\kappa)\varphi = \lambda\varphi$ corresponding to $\lambda = 2|\xi + \chi|\cos\theta$ is given by

$$\varphi_n = e^{in\tau}\left[e^{i\theta|n|} + S_\kappa(\lambda)e^{-i\theta|n|}\right]$$

where

$$S_\kappa(\lambda) = -\frac{\lambda - \Psi(\kappa) - 2|\xi + \chi|e^{i\theta}}{\lambda - \Psi(\kappa) - 2|\xi + \chi|e^{-i\theta}}.$$

Here $\theta \in [-\pi, \pi]$ is the quasimomentum corresponding to direction transverse to the diagonal. The reflection coefficient S_κ has the pole on the physical sheet in λ-variable which corresponds to eigenvalue (2). Since Q_χ is the rank 1 perturbation of standard Jacobi matrix this pole is the only singularity of S_κ on the Riemann surface of the energy λ.

2.3 Effective Masses and Fit of the Parameters

Using (2) one can now calculate explicitly the effective masses at the ends of the polaron zone by the formula $m = \frac{1}{\lambda''(\kappa)}\Big|_{\kappa=\kappa_0}$ provided $\lambda'(\kappa_0) = 0$. The result is

$$m = \left.\frac{\sqrt{\Psi(\kappa)^2 + 4(1 + \xi^2 + 2\xi\cos\kappa)}}{\Psi'^2 + \Psi\Psi'' - 4\xi\cos\kappa}\right|_{\kappa=\kappa_0}$$

where κ_0 is defined by the equation

$$\Psi(\kappa_0)\Psi'(\kappa_0) = 4\xi\sin\kappa_0.$$

The case $\Psi(\kappa) = const$ or $\Psi_\tau = \psi\delta_{\tau,0}$ comprises a precise discrete analog of the interaction suggested in the paper [2]. The corresponding polaron zone is $\sigma_{pol} = \left[\sqrt{\psi^2 + (|\xi| - 1)^2}, \sqrt{\psi^2 + (|\xi| + 1)^2}\right]$ for $\psi > 0$ and $-\sigma_{pol}$ for $\psi < 0$. The coupling constant ψ here is an analog of the Frölich constant α [1]. This constant is incorporated in the Frölich hamiltonian H as $H = H_0 + \sqrt{\alpha}V$, where H_0 is the operator of kinetic energy of electron-phonon system and V is the operator of electron-phonon interaction. In the limit of weak coupling $\psi \sim 0$ by (2) we have $\lambda - \lambda_0 \sim \frac{1}{4|\chi+\xi|^2}\psi^2$, where $\lambda_0 = 2|\chi + \xi|$ is the rest of the zone corresponding

to scattered waves. Comparing this with the asymptotic $\Delta\lambda \sim \alpha$ of the polaron energy measured from the rest of the continuous spectrum known from physical literature [3] one takes $\psi = \tilde{C}\sqrt{\alpha}$, $\tilde{C} = 2|\chi + \xi|$.

Then we have $\sin\kappa_0 = 0$ what gives $\kappa_0 = \pi$ for minimum. Thus

$$m = \frac{\sqrt{\psi^2 + 4(1-\xi)^2}}{4\xi}. \tag{4}$$

At $\psi \sim 0$ the polaron effective mass (4) should coincide with the electron effective mass which is 1 in the accepted system of units. This condition fixes the parameter ξ as $\xi = \frac{1}{3}$. This defines completely $\tilde{C}$ at the rests of the polaron zone.

Let us note that the Frölich constant α can be expressed in terms of the physical characteristics of the material [4]

$$\alpha = \frac{1}{2}\left(\varepsilon_\infty^{-1} - \varepsilon_0^{-1}\right)\frac{e^2}{\hbar\omega_0}\left(\frac{2m_e^*\omega}{\hbar}\right)^{\frac{1}{2}}$$

where ε_0 and ε_∞ are dielectric constants at zero and high frequencies, m_e^* is the electron effective mass. Thus we conclude that the coupling constant ψ is completely fixed by the choice of the material. As both of the parameters ψ and ξ are fitted one can calculate the polaron effective mass (4) for various materials.

In the weak coupling limit $\psi \sim 0$ electrons practically do not interact with the lattice phonons. Vice versa, in the strong coupling limit $\psi \to \infty$ electrons strongly interact with the lattice phonons. In this case the description of the electron-phonon interaction in the frame of field theory becomes essentially nonlinear. This means that the linear approximation we used is not suitable in this regime. That is the reason why the asymptotics $\lambda \sim \sqrt{\alpha}$, $m \sim \sqrt{\alpha}$ at $\psi \to \infty$ obtained from (2) under the accepted fit of ψ differ from the physically expected $\lambda \sim \alpha^2$, $m \sim \alpha^4$ [5].

Note that when $\xi = 0$ the polaron zone degenerates into the point $\lambda = \sqrt{\psi^2 + 4}$. This point is the infinitely degenerated bound state of L. One can interpret this as the result of braking the electron by vacuum of infinitely heavy phonons.

3 Conclusion

The suggested model of electron-phonon interaction demonstrates on qualitative level the rising of polaron branch in the spectrum of the Hamiltonian under consideration while the spectrum of scattered waves remains the same as for unperturbed problem. This model leads to the explicit formula for the polaron effective mass. The latter makes possible to fix the model parameters ψ and ξ as it is described above. Being applied to the description of the electron propagation through a quantum wire in non-ballistic regime the model allows to calculate the effective mass of charge carriers in terms of ψ and ξ. It opens the way for estimation of the contribution of electron-phonon interaction into the conductivity in the working regime of any nanoelectronic device based on quantum wires. The simplest such device is the quantum wire with the periodic external voltage applied [6, 7, 8, 12, 13, 11, 12, 13, 14, 15, 16, 17]. As it is has been shown [6, 7, 8, 12, 13] in the effective mass of charge carriers is important characteristic of devices based on Mott-Peierls stimulated transition and could change the upper limits for the temperature and gate voltage applied.

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